The Influence of Strain on the Microwave Dielectric Properties of $(Ba,Sr)TiO_3$ Thin Films

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Abstract

•Perovskite thin films grown by PLD are oxygen deficient and the lattice of expands beyond the size reported for fully oxidized material.

•Post-deposition annealing films in an O_2 can be used to fill some of these vacancies, which results in a reduction in the lattice parameter.

•Epitaxial BST films deposited onto (001) MgO by pulsed laser deposition (PLD) show a large tetragonal distortion (ratio of in-plane and surface normal lattice parameters, D = *a/c*). The distortion depends on the oxygen deposition pressure (i.e., the number of oxygen vacancies).

•A strong correlation is observed between the magnitude of the tetragonal distortion and the microwave dielectric properties, measured at 1-20 GHz.

•BST films with a small distortion (i.e, D~1) have higher dielectric constants and lower dielectric loss compared to films with a large distortion.

•The variation of the microwave properties with the film structure can be attributed to strain induced changes in the polarizabilty in the film.

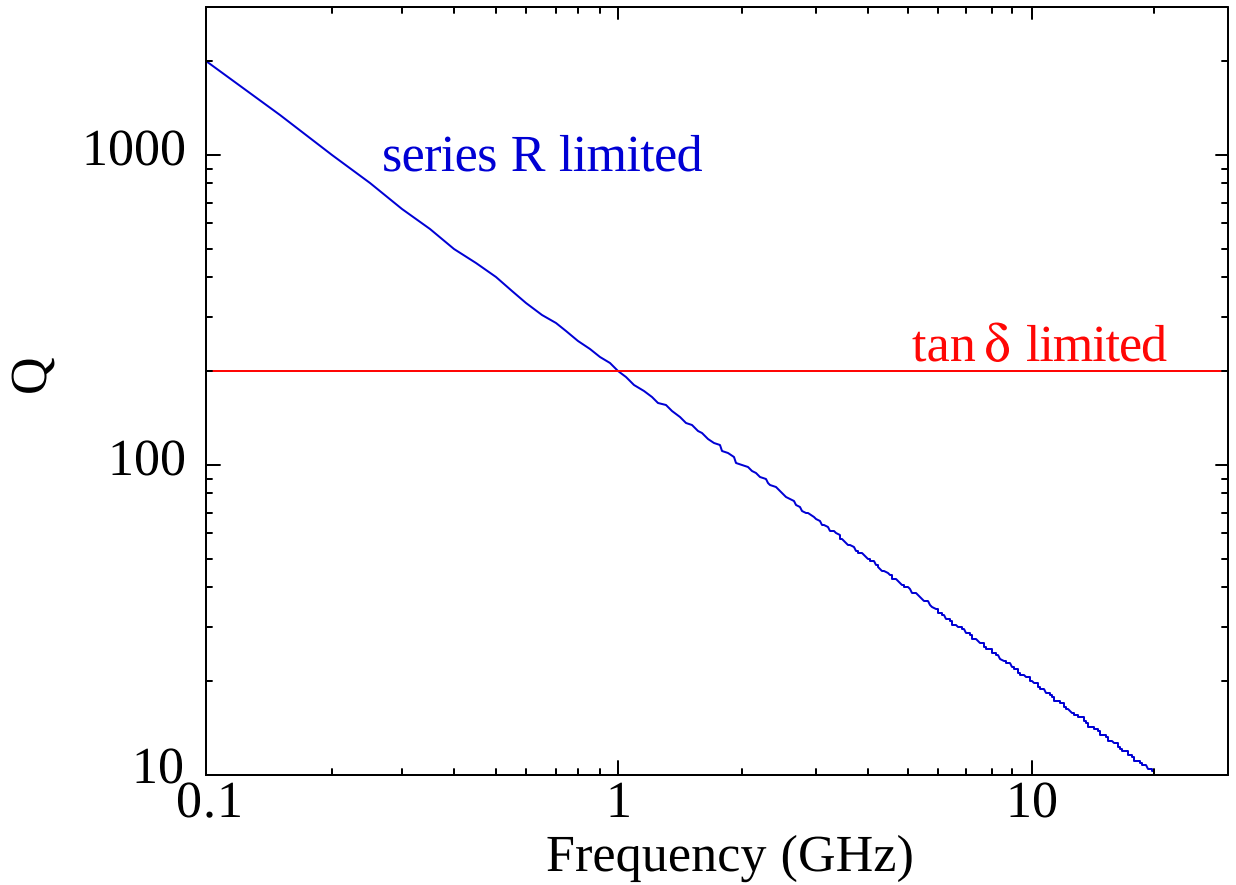
• BST films grown by PLD at an oxygen deposition pressure of 50 mTorr, exhibit a minimum distortion and a maximum figure of merit (Q x %Tuning).

Prior Art

- Most Tuned RF Circuits Rely on a Variable Capacitance Device (GaAs Varactor)
- Capacitance Change in a Semiconducting Varactor Arises from Changes in the Depletion Region of the Junction Diode.
- As Bias is Increased, Depletion Region is Enlarged, Leading to a Voltage Dependent Capacitance.
- GaAs Suffer from a Number of Disadvantages:
  - Power Consumption
  - Joule Heating
  - Inherently Lossy, Especially at High Frequencies

To Improve Systems Performance at High Frequencies will Require New Device Architectures

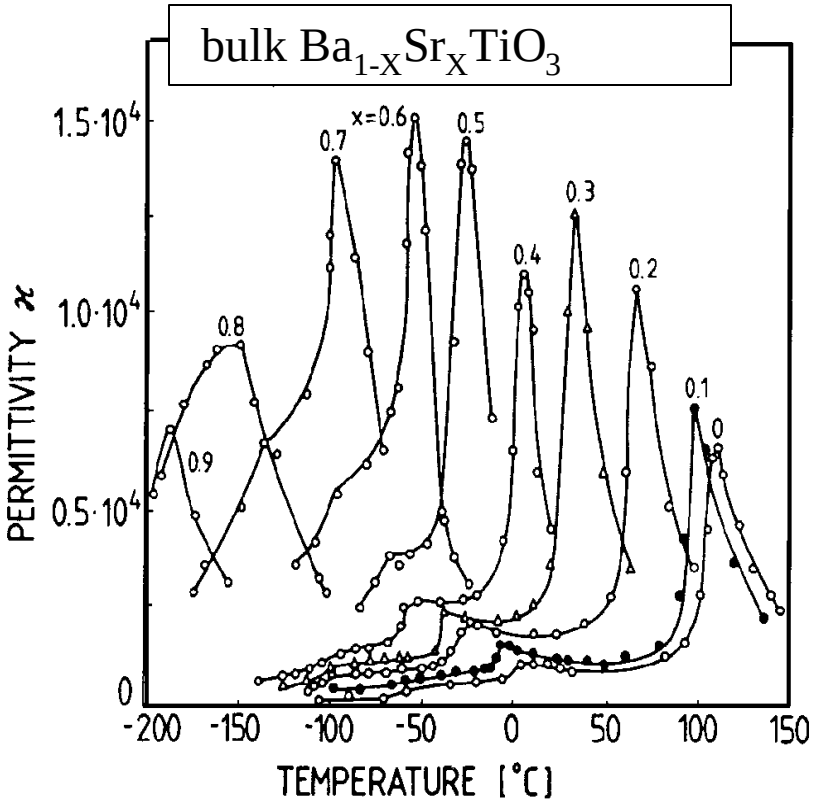
Comparison of the Frequency Dependencies of tanδ Limited and series R limited Capacitors

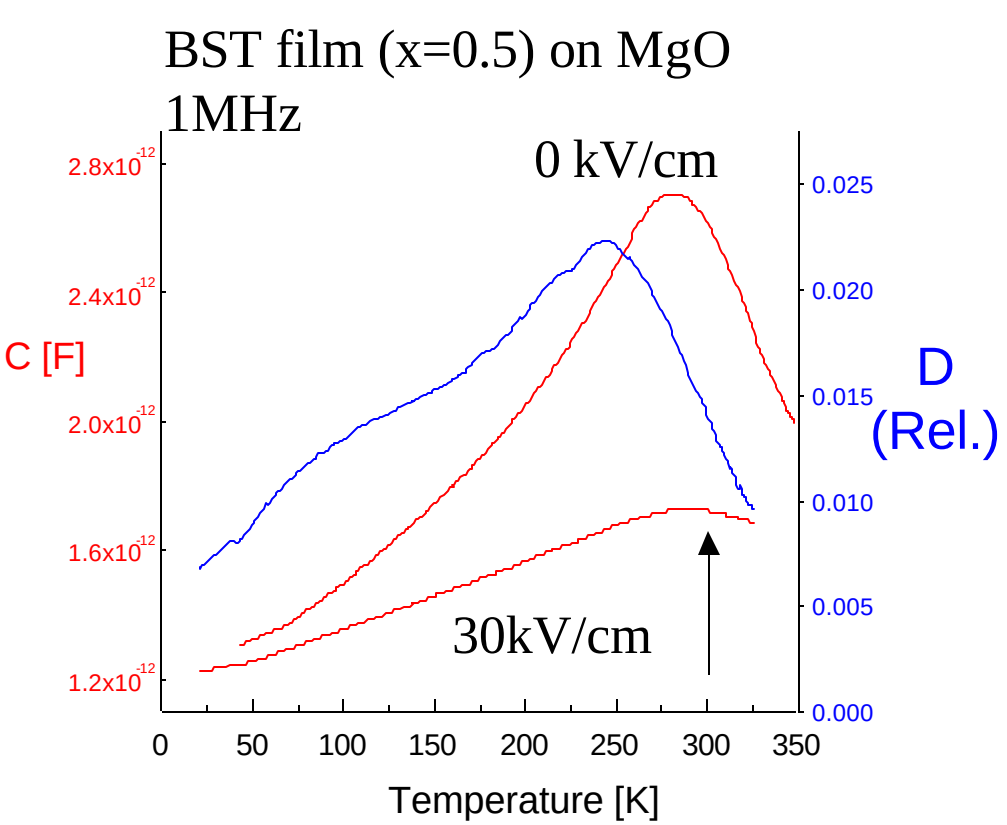


Benefit to Using Ferroelectric Devices Increases at Higher Frequencies

$Ba_{1-X}Sr_XTiO_3$

Ferroelectric Properties Depend on Composition and Temperature



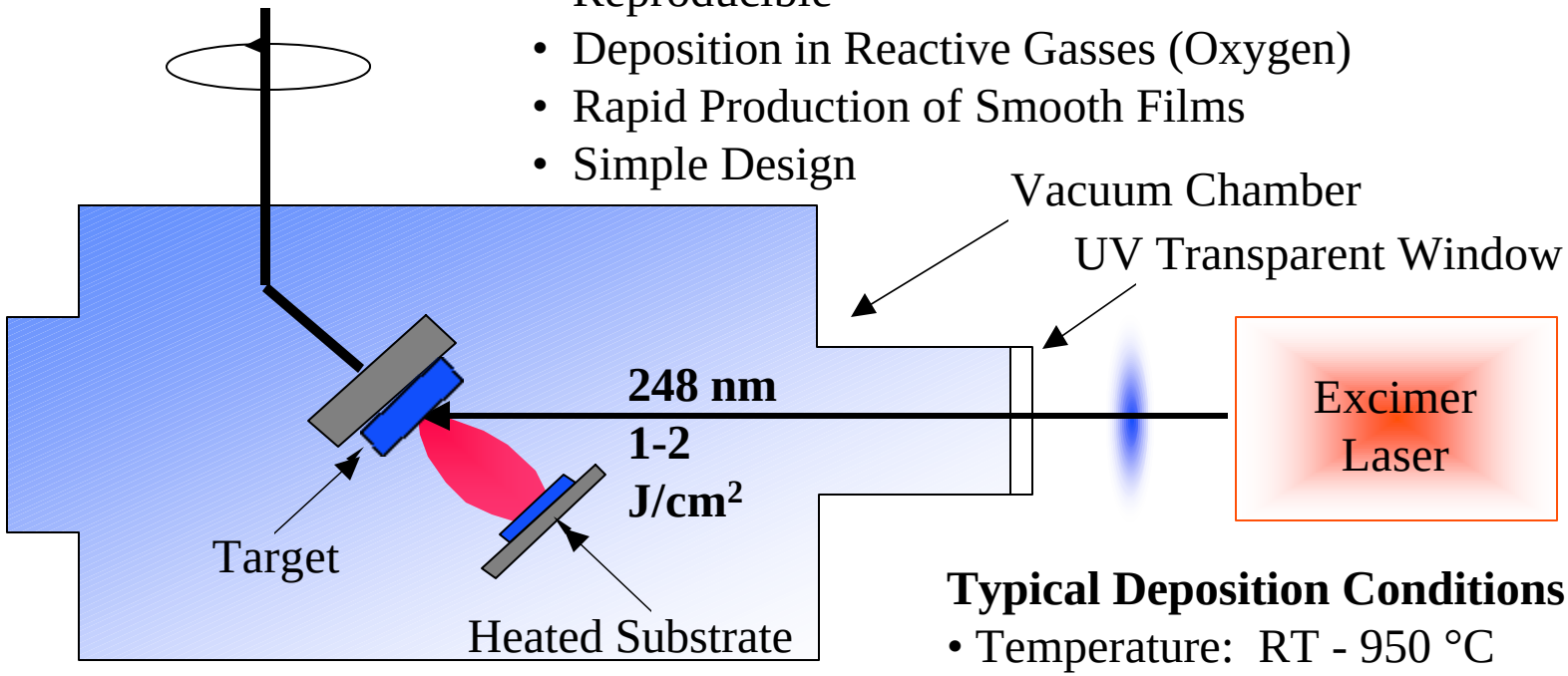


- Dielectric Tuning and Loss are Strongly Correlated
- Regions with Large Tuning and Low Dielectric Loss Exist

Introduction to PLD

Technique Offers Many Advantages:

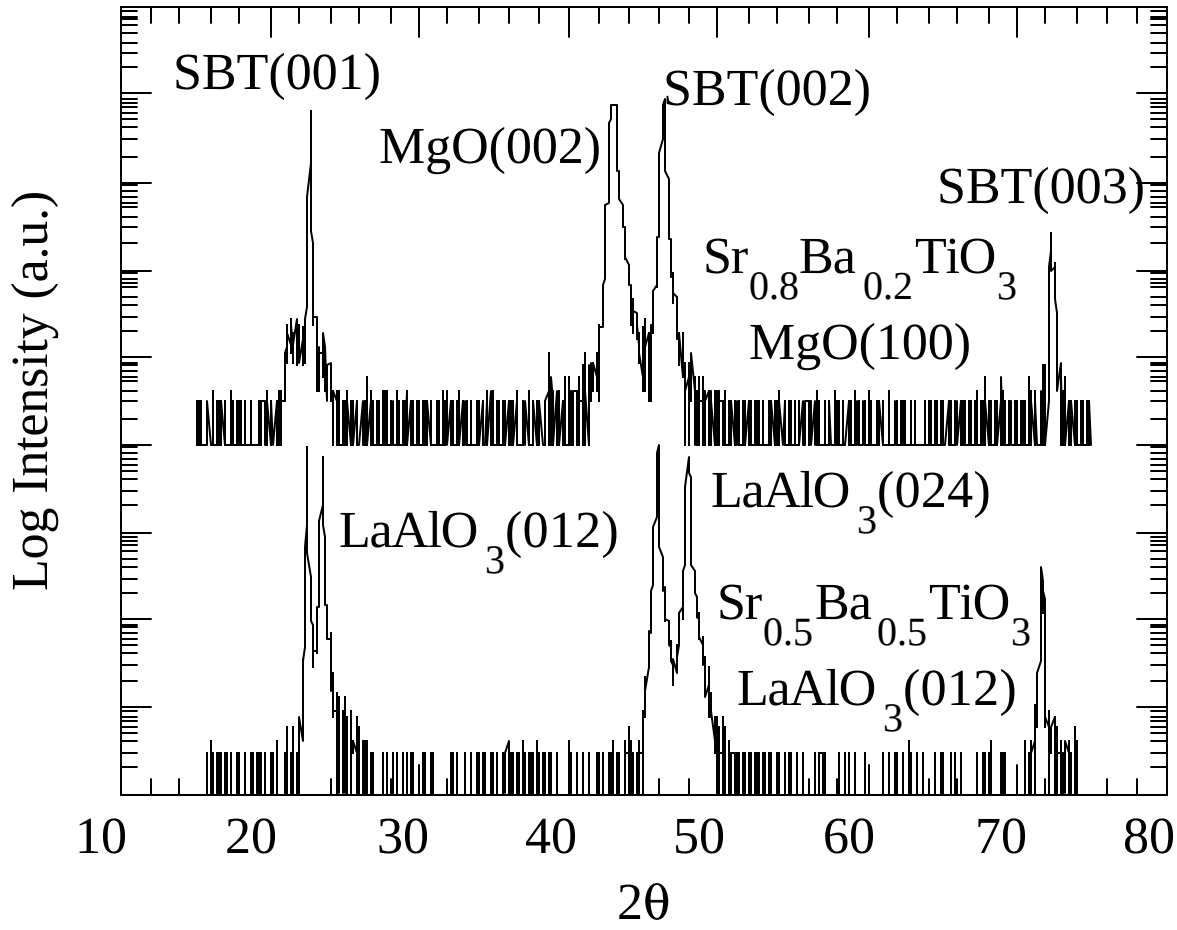
- Transfer of Pellet Stoichiometry
- Reproducible
- Deposition in Reactive Gasses (Oxygen)
- Rapid Production of Smooth Films
- Simple Design



Typical Deposition Conditions:

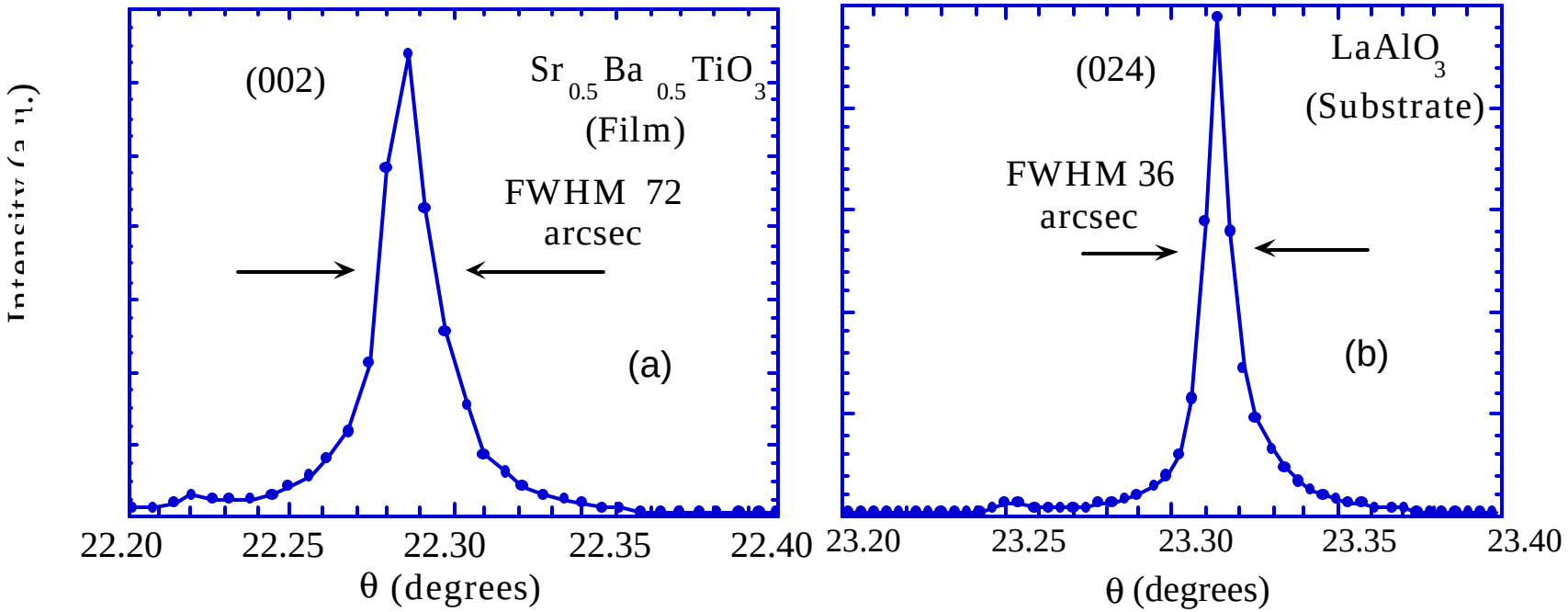
- Temperature: RT - 950 °C
- Pressure: 10^{-7} - 1 Torr
- Deposition Rate: 0.1 - 10 Å/sec

X-Ray Diffraction from $Sr_xBa_{(1-x)}TiO_3$ Thin Films



- As deposited Films are Single phase and exclusively (001) oreinted.

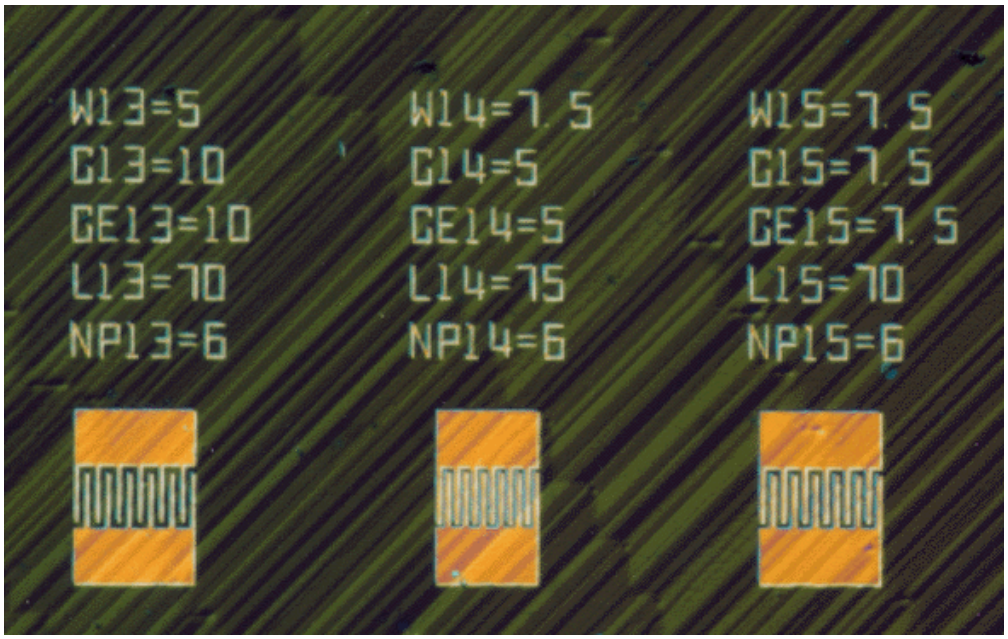
X-Ray Rocking Curves for Pulse Laser Deposited SBT Fi Comparable to MBE Quality

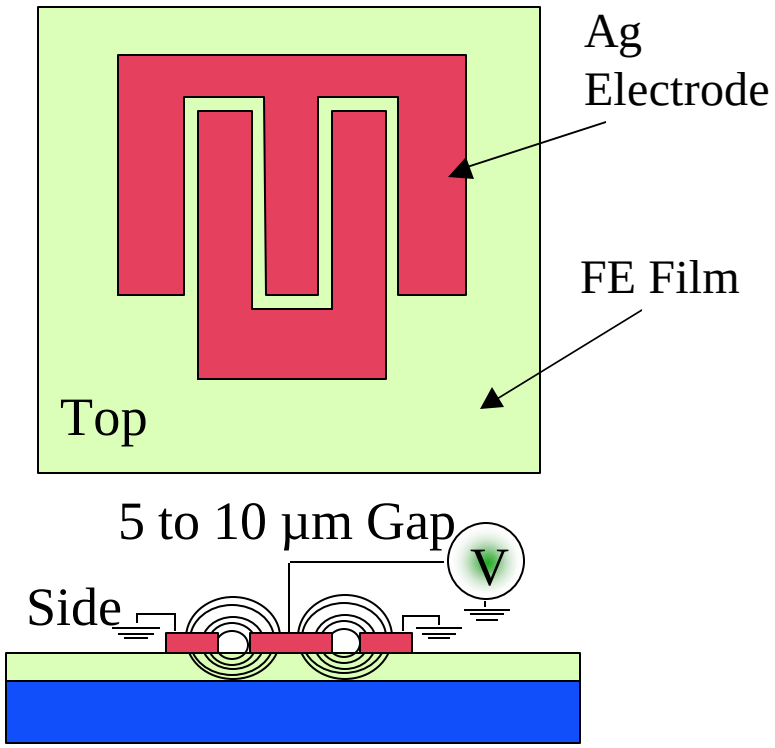


"X-ray characterization of extremely high quality(Sr,Ba)TiO $_3$ films grown by pulsed laser deposition"

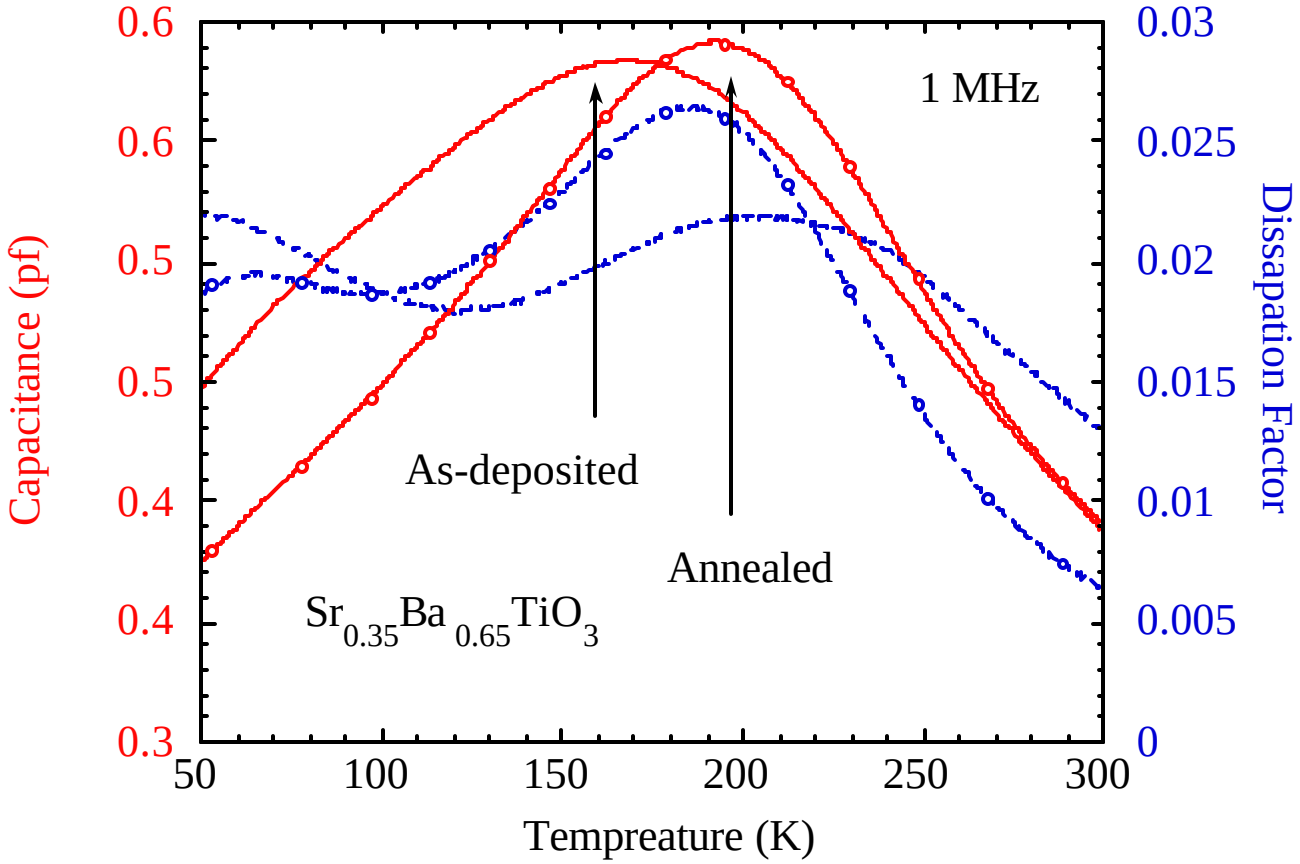
Qadri, S. B.; Horwitz, J. S.; Chrisey, D. B.; Auyeung, R. C. Y.; Grabowski, K. S. Appl. Phys. Lett., 66(13), 1605-7 1995.

Dielectric Properties Measured Using Interdigitated Capacitor



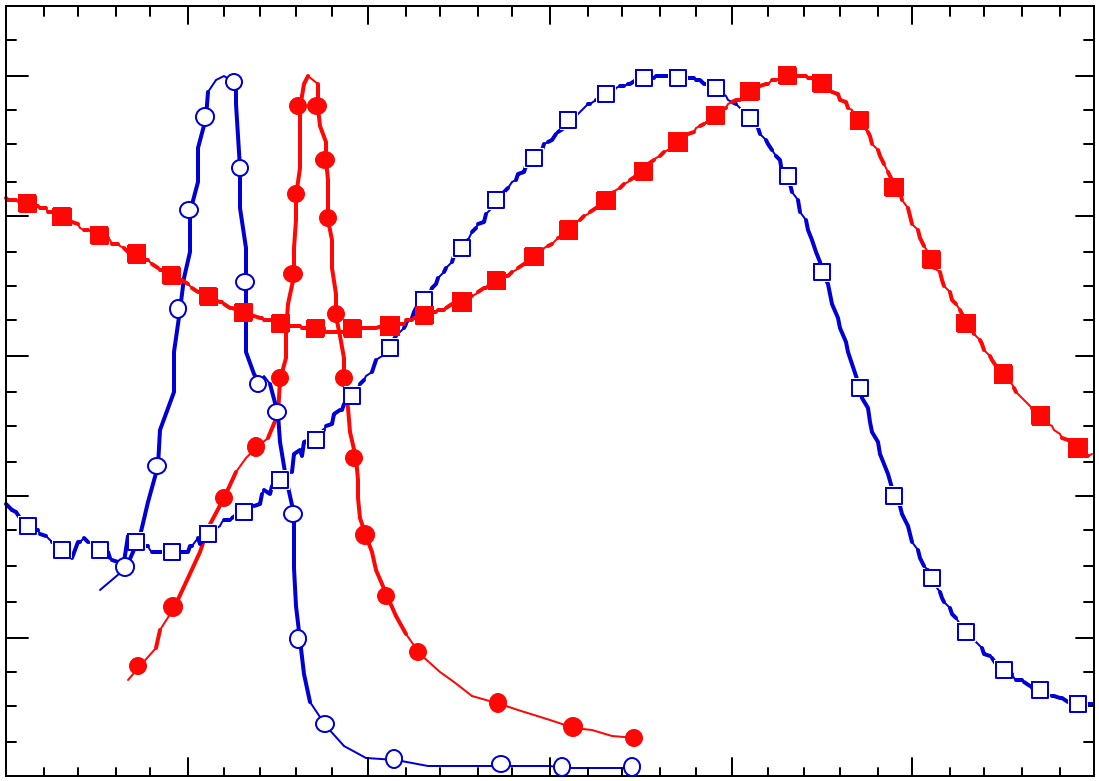


Oxygen Vacancies



- From XRD, as deposited films are oxygen deficient
- Post-deposition annealing can fill ***some*** of the oxygen vacancies
- Filling of oxygen vacancies leads to a reduction in the dielectric loss

Dielectric Constant and Dissipation Factor for $Ba_xSr_{(1-x)}TiO_3$



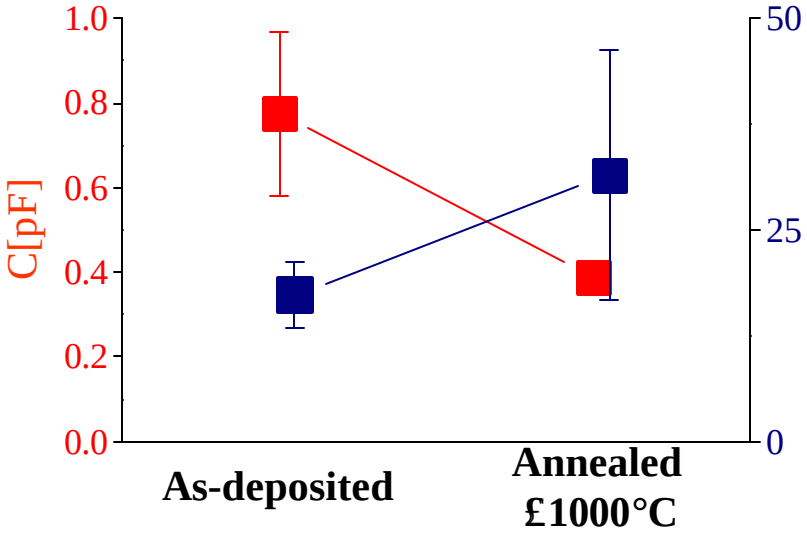
- Broad dielectric properties in thin correspond to electrically inhomogenious material

Dielectric Properties of BST Films (1-20GHz)

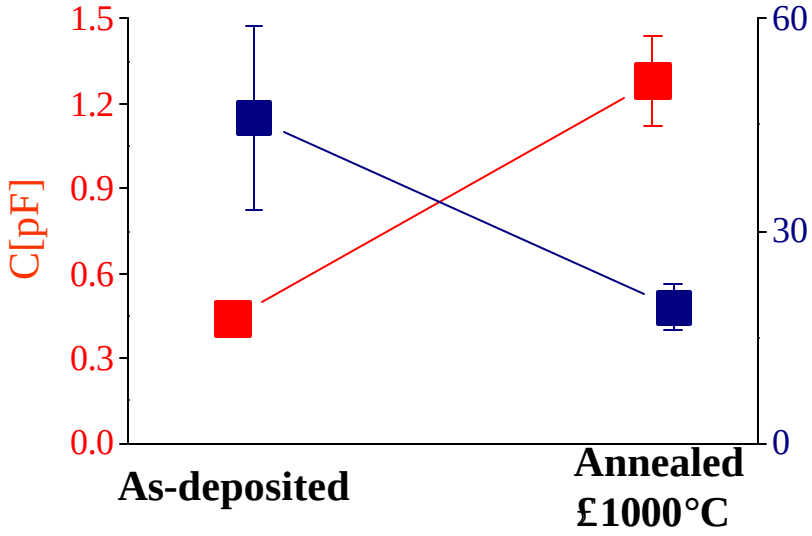
	Typical		Maximum	
substrate	MgO	LAO	MgO	LAO
film dielectric constant	1000	1500	2973	3328
tuning [%] @67 kV/cm	30	50	62	75
Q	45	25	100-250	50-70
Tanδ	0.022	0.040	0.010 - 0.004	0.020-0.014

Strain Creates an Inverse Relationship Between Tunability and Loss at Microwave Frequencies in Epitaxial Films

BST on MgO

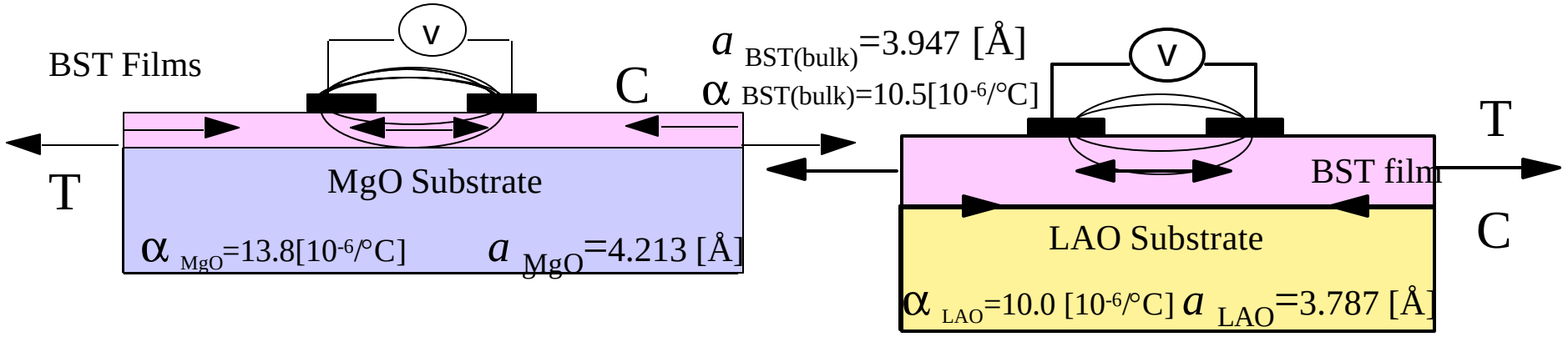


BST on $LaAlO_3$



- As deposited films on MgO are in tension as deposited, and in compression after annealing in O_2.
- As deposited films on $LaAlO_3$ are in compression as-deposited, and in tension after annealing in O_2.
- In strained films, we observe an inverse relationship between tunability and dielectric loss.

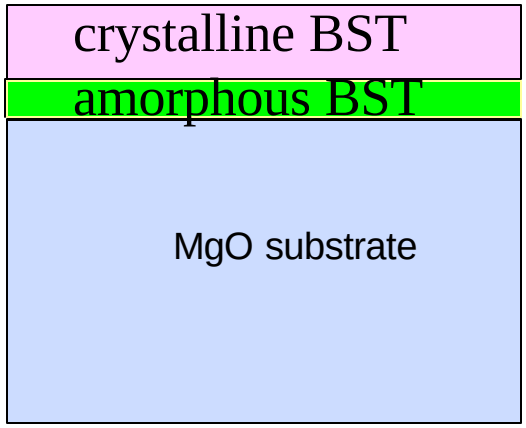
Strain Effect of epitaxial BST film on the dielectric properties

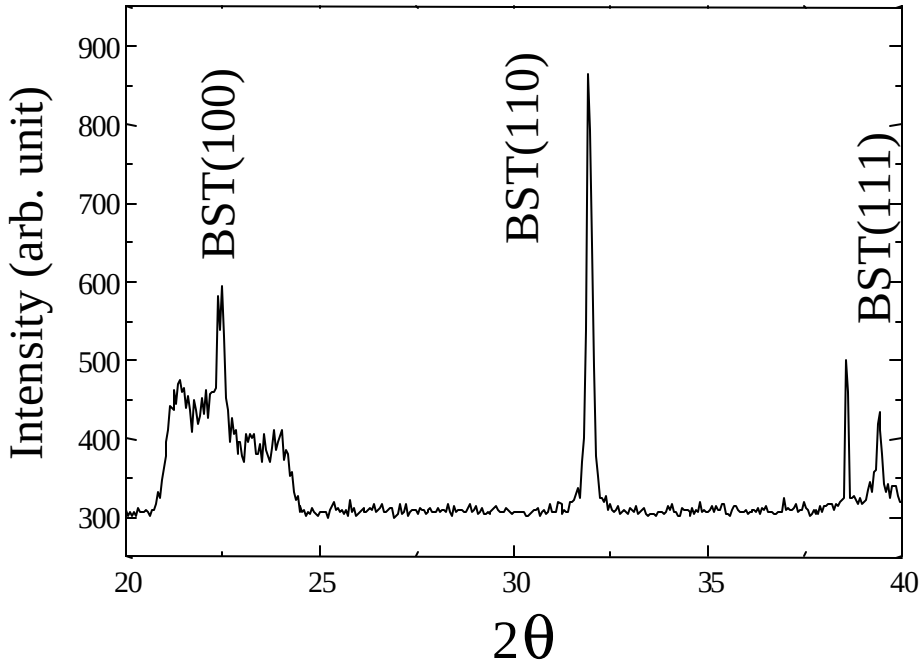


- Strain due to lattice mismatch and the difference in thermal expansion coefficients between film and substrate
- BST Films grown directly on dielectric substrate are Highly Oriented and Highly Strained.
- Coupling of Strain and Electric field makes Film properties significantly different from bulk material.

Strain Free BST Film

1. Deposit BST at room temp. (~5 nm): amorphous layer
2. Deposit BST at 750^{o}C (~495 nm): crystalline layer

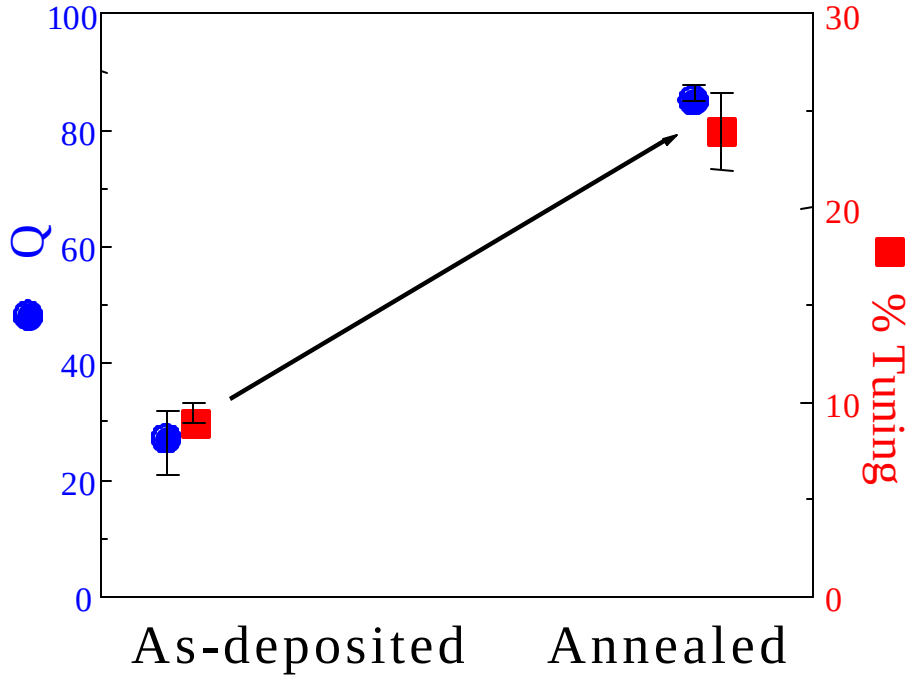




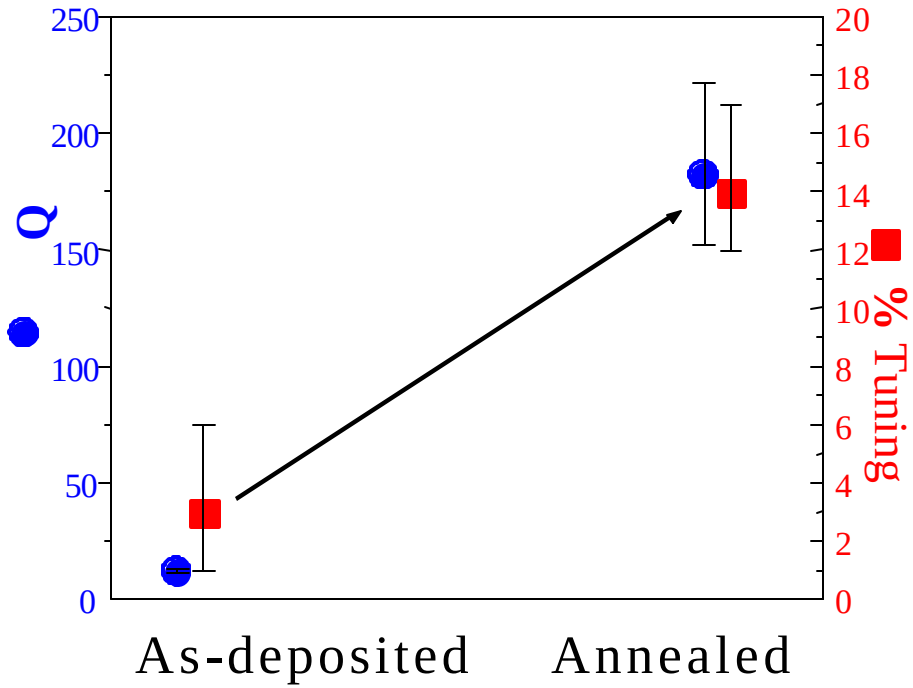
Produce a strain free BST film (lattice constant a = 3.9606 Å)

Strain-Relieved BST/MgO

1% Mn doped BST on MgO



1% W doped BST on MgO

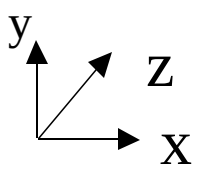


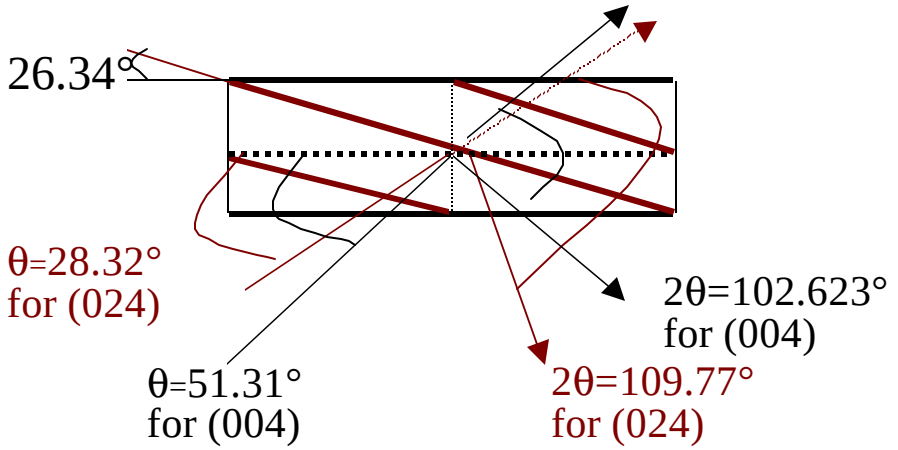
Both Q and % Tuning are Increased

Lattice parameters of Epitaxial BST Film determined by symmetric and asymmetric θ-2θ XRD scans

Symmetric θ-2θ scan for (004) diffraction

Asymmetric θ-2θ scan for (024) diffraction



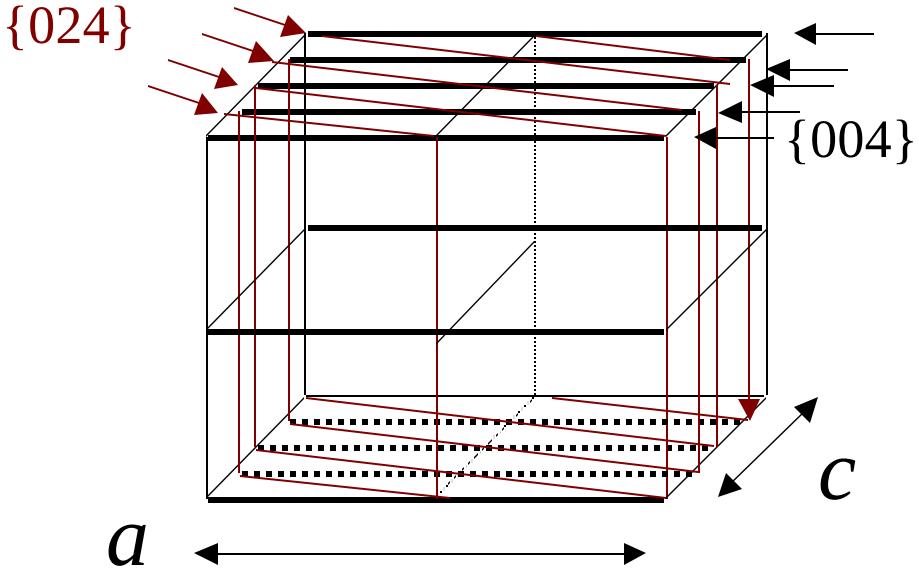


$$d_{hkl} = h^2/a^2 + k^2/a^2 + l^2/c^2$$

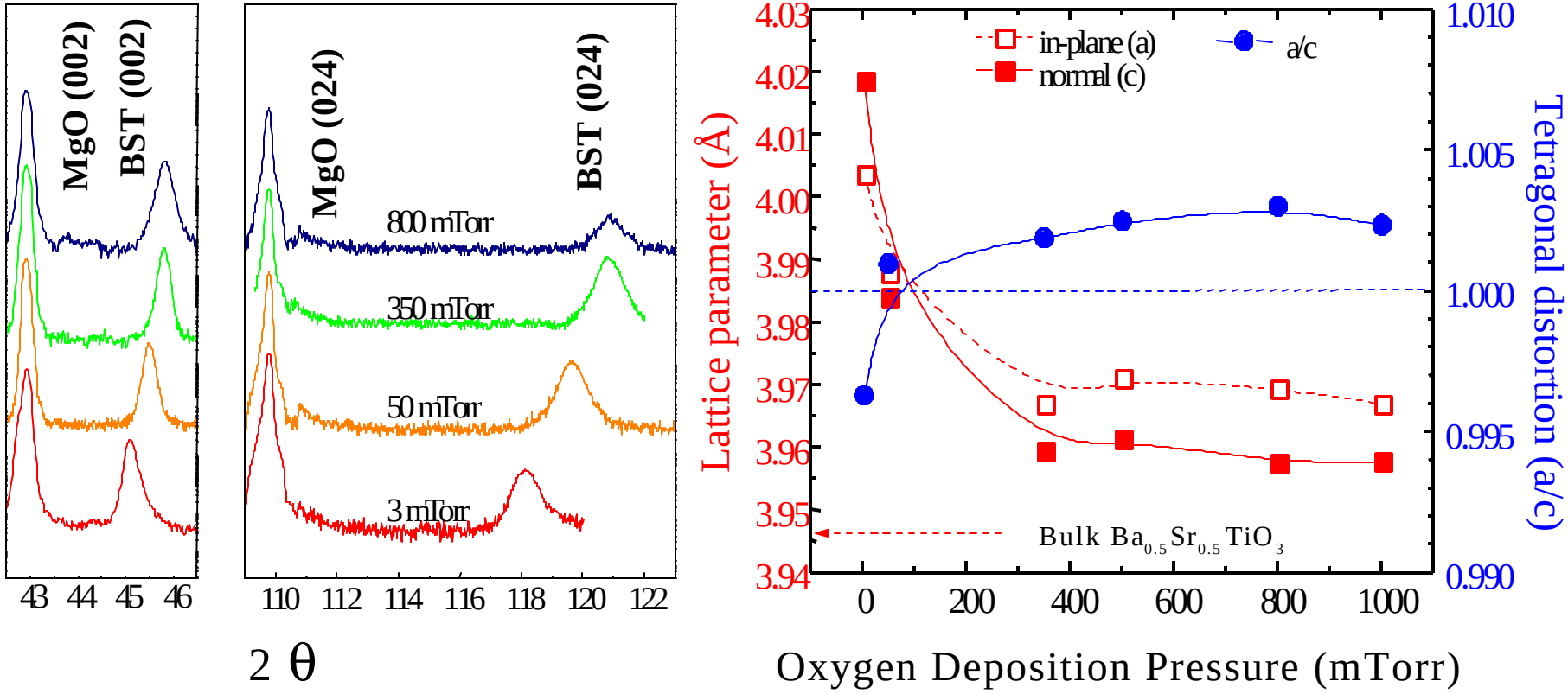
$$(n)\lambda = 2d\sin\theta$$

2 knowns from XRD : d_{004}, d_{024}

2 unknowns : a, c



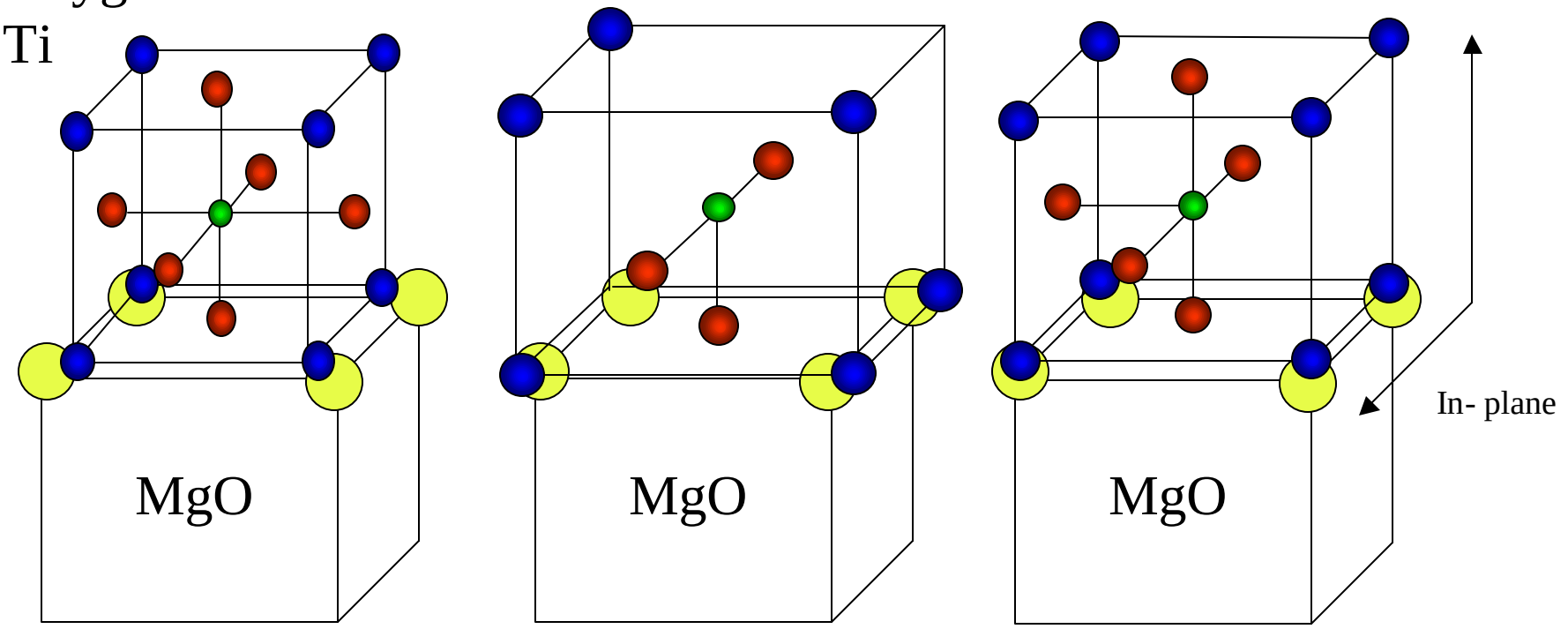
Heteroepitaxial Films Deposited by PLD are Highly Strained



- c > a below 3 mTorr, c ~ a at 50 mTorr, c < a over 150 mTorr
- Lattice parameter of BST film > Lattice parameter of the Bulk

Defect Mediated Strain Reduction in Epitaxial Films

- Ba,Sr
- Oxygen
- Ti



Stoichiometric Oxygen: **Strained-Compression**

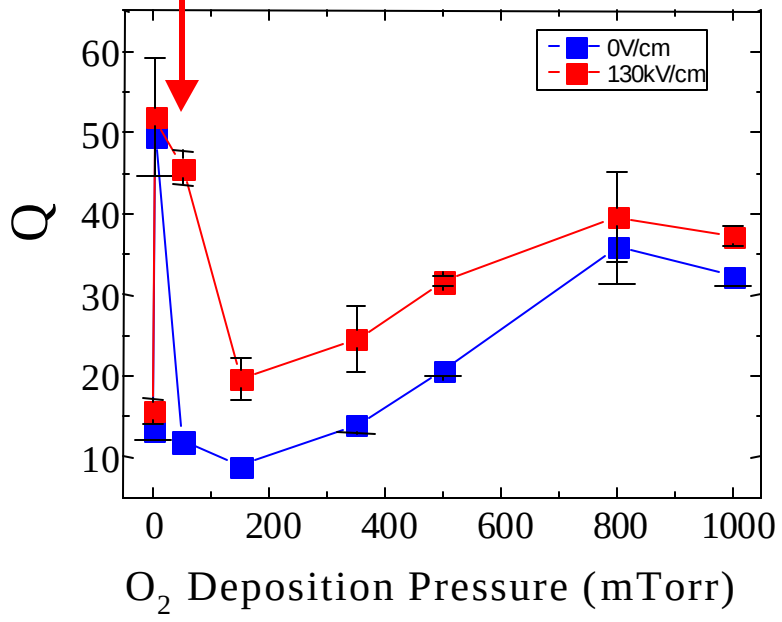
Sub-stoichiometric Oxygen: **Strained-Tension**

Slightly sub-stoichiometric Oxygen: **No Strain**

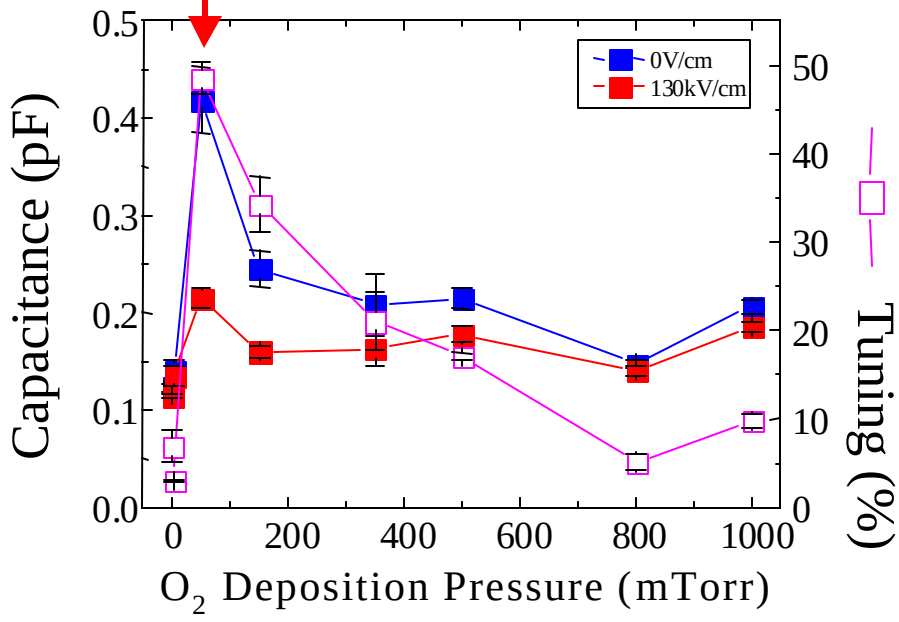
- Careful control of oxygen deposition pressure can be used to minimize film in-plane strain and improve tunable microwave dielectric properties.

Effect of Oxygen Pressure on Microwave Dielectric Properties

Quality factor Q = 1/ tan δ



C and %Tuning



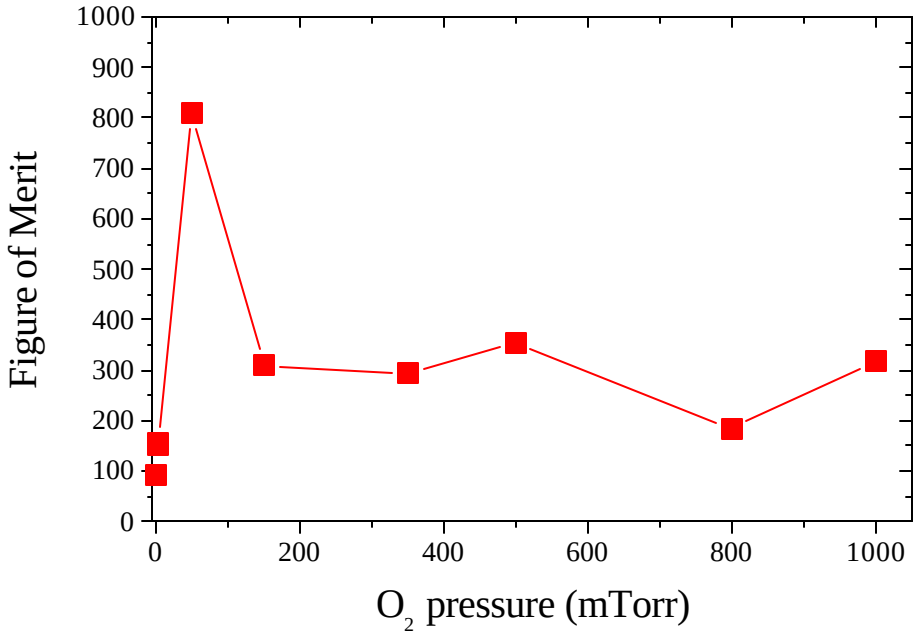
- The film with a minimal stress (a = c) shows
  → High quality factor Q and High Dielectric tuning at the same time

Oxygen pressure effect on dielectric properties of $Ba_{0.5}Sr_{0.5}TiO_3$

Figure of Merit

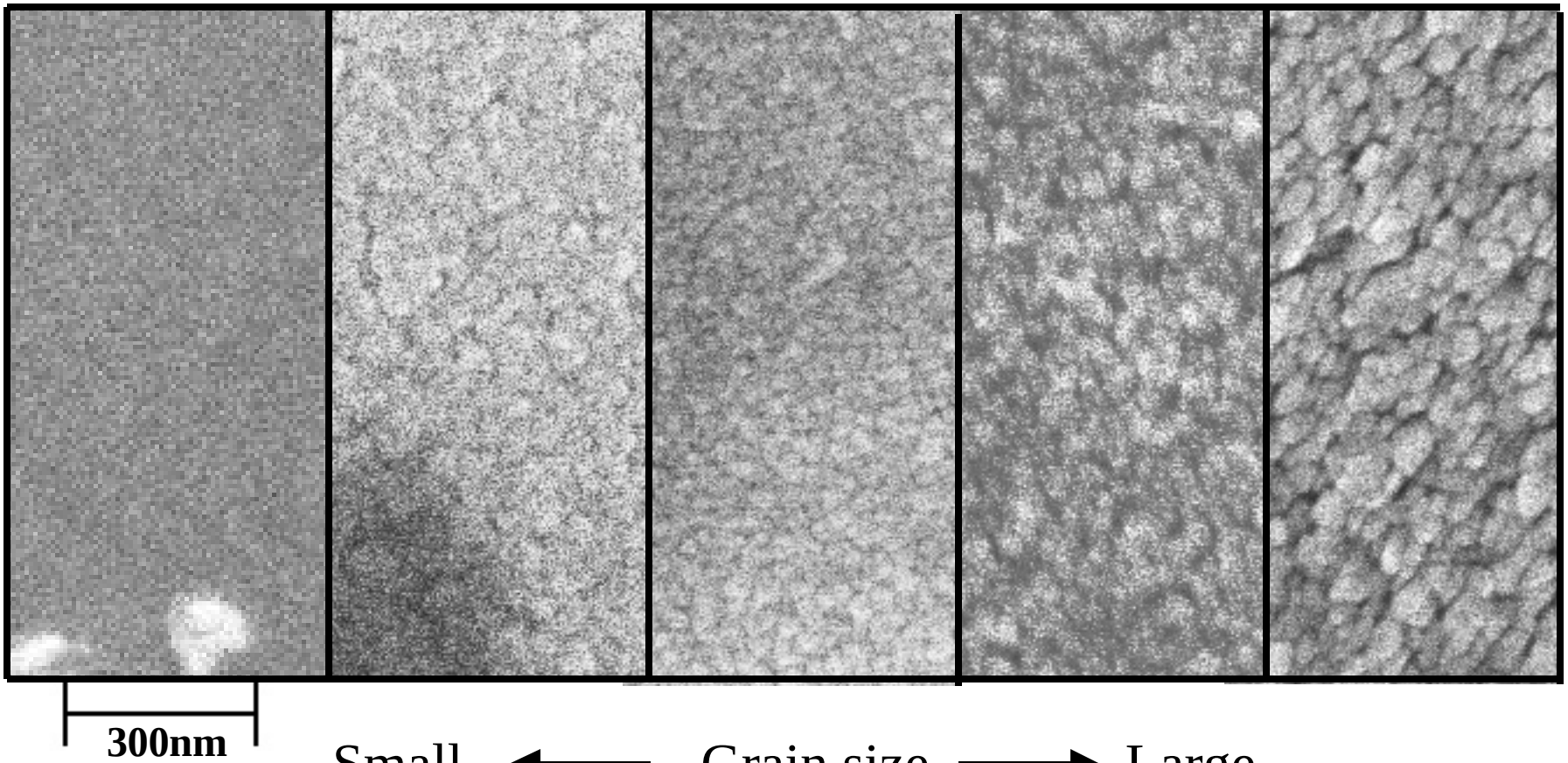
K= $\%T_{(0V:40V)} \times Q_{0V}$

K= $\%T_{(10V:40V)} \times Q_{10V}$

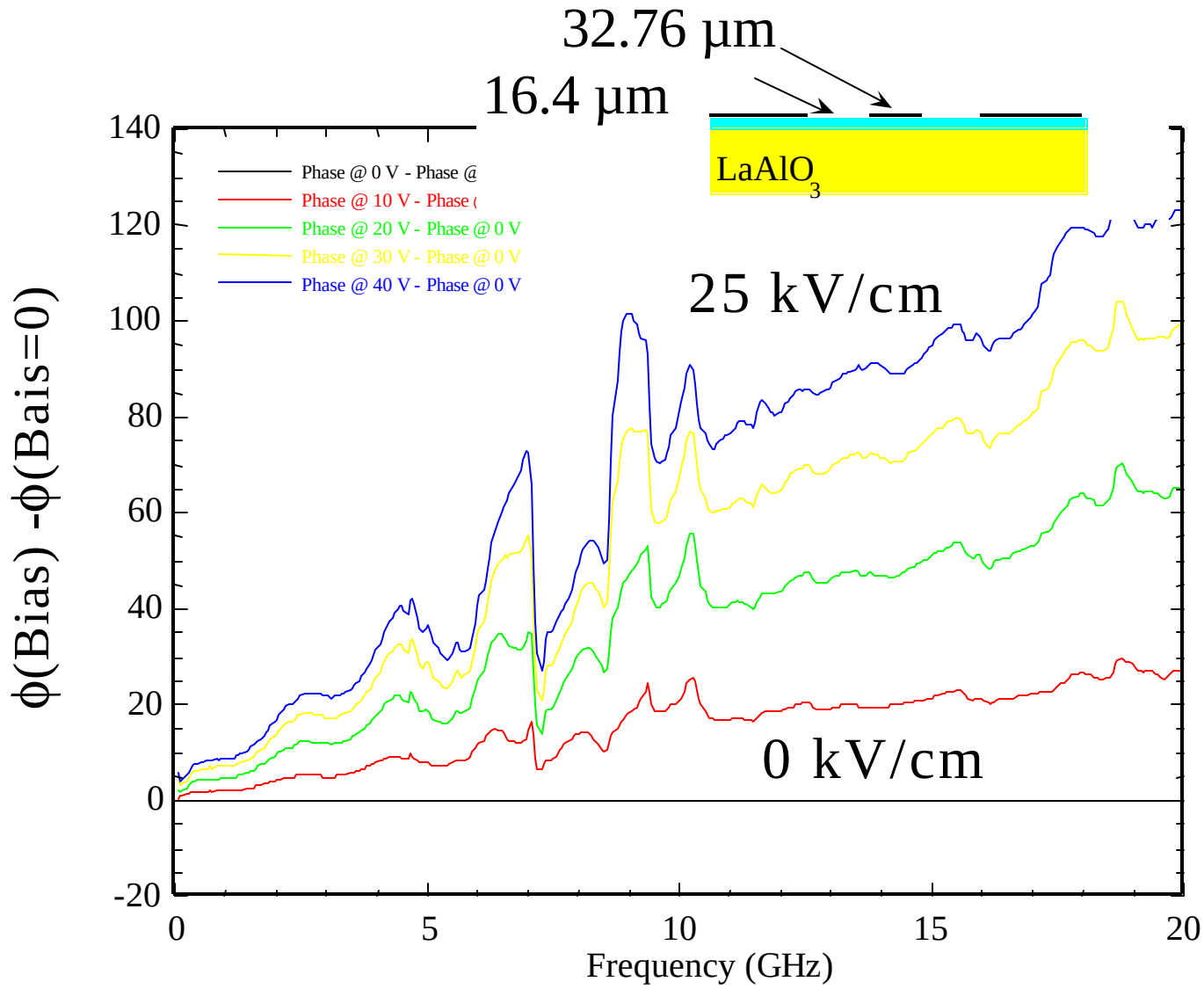


- The film with a minimal stress (a = c) shows Highest Figure of Merit

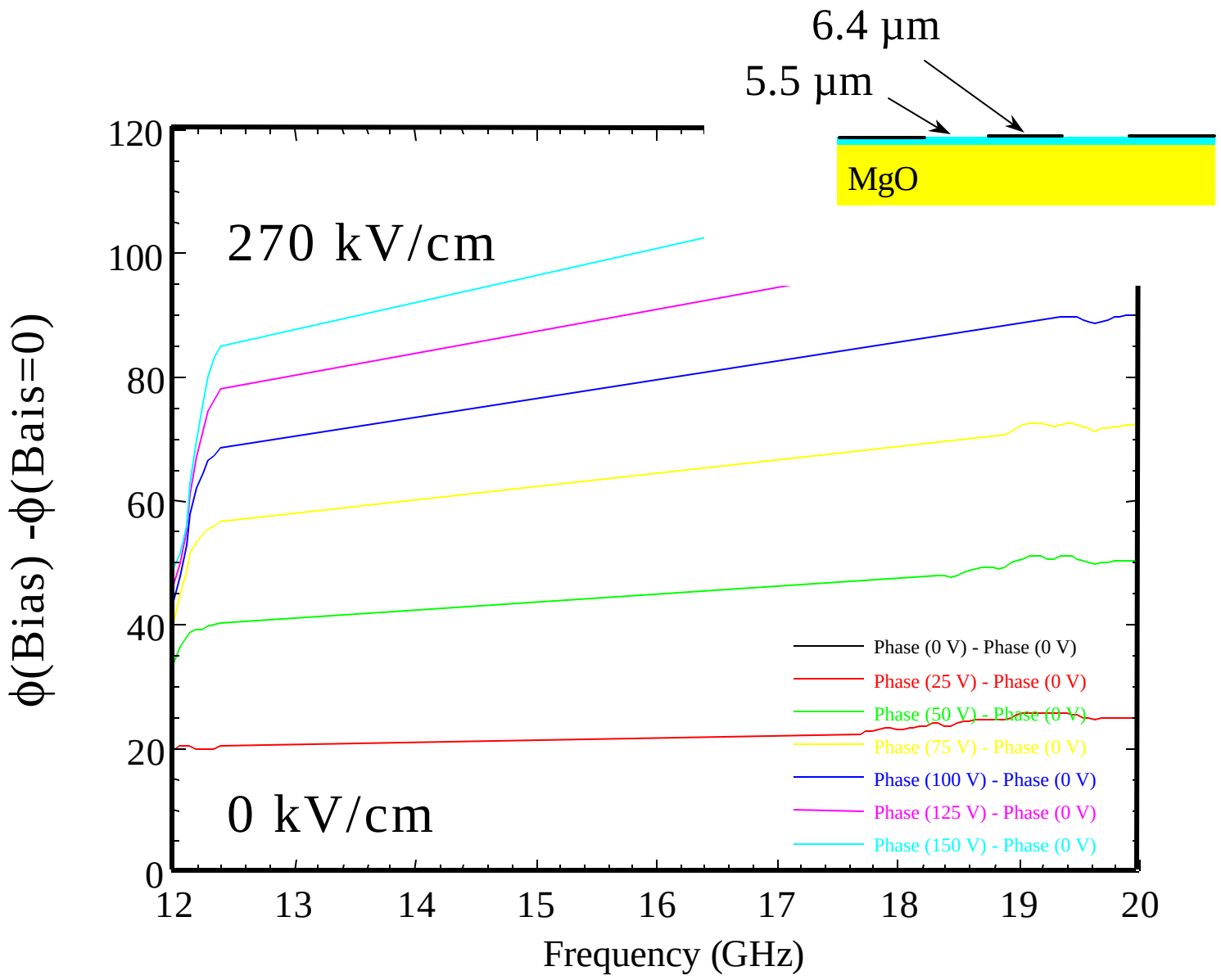
SEM image of BST50 on MgO with different O_2 pressure



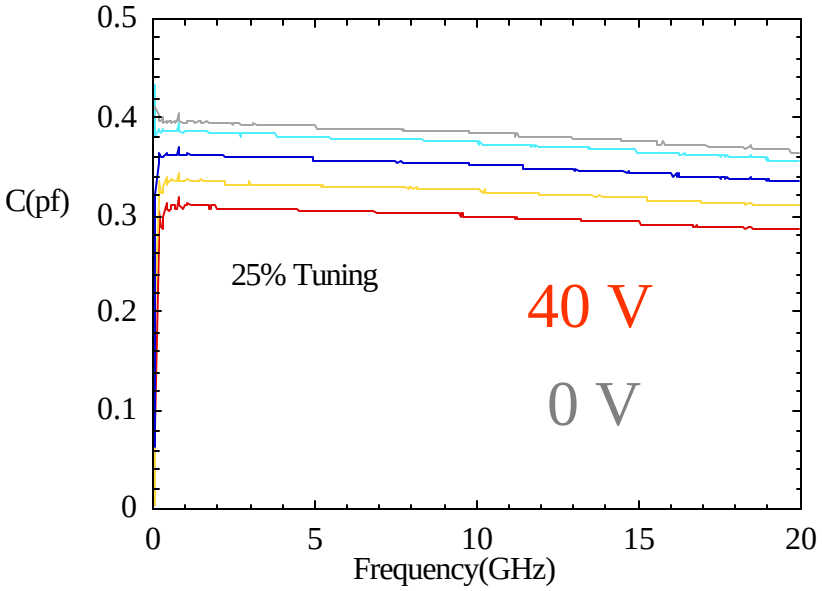
Phase Difference as a Function of Frequency and Bias for a 1-cm Coplanar Waveguide Transmission Line

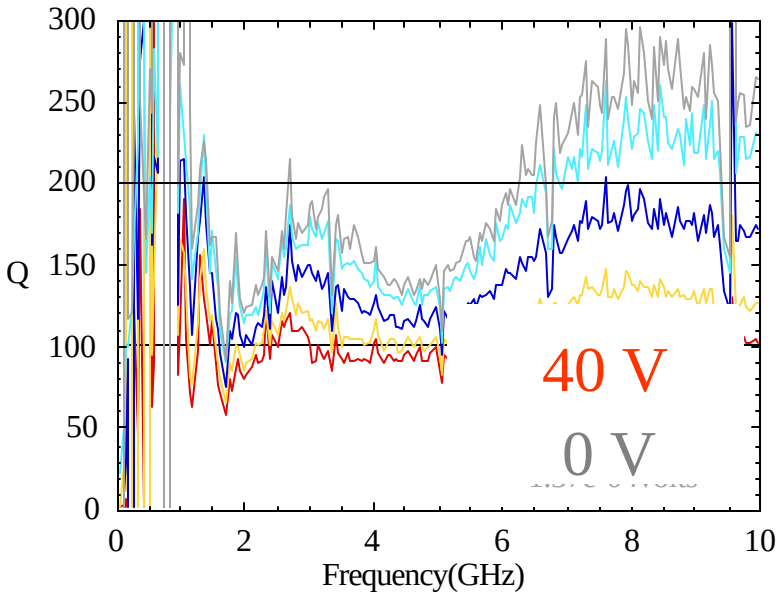


Phase Difference as a Function of Frequency and Bias for of 1-cm Coplanar Waveguide Transmission Line



Current State of the Art for Ferroelectric Thin Film





- Q > 200 at 10 GHz with 25 % Tuning.

Summary

- BST thin films, deposited by PLD are currently being used to develop microwave tunable oscillators and phase shifters.
- Epitaxial films deposited on non-lattice matched substrates are highly strained. Film strain has a strong influence on dielectric constant, tunability and dielectric loss.
- Strain relieved films have been generated by using amorphous buffer layers and by varying the number of oxygen vacancies.
- Strain relieved films have a higher figure of merit for applications in tunable microwave circuits.